中心实验室仪器使用心得专栏 III 期 飞行时间质谱仪

基本信息

主要应用

成果展示

-----投稿人：刘敏

- **仪器型号：** WatersVionIMS Qtof
- **主要附件：** 与Waters UPLC H-class 联用，配备UNIFI控制软件及代谢组学数据分析QI软件。
- **主要参数:**

1.四极杆质量范围： m/z 20-8,000; TOF质量范围：m/z 20-100,000。

2. 分辨率：≥40,000 FWHM

3. 质量精确度，外标法MS及MS/MS模式达到<1 ppm。

4. 灵敏度（全扫描模式）：1 pg利血平，柱上进样，MS模式下，30张图谱/秒的采样速率下，S/N ≥ 15000:1。

5. 谱图内动态范围：5个数量级。

6. 数据处理系统：仪器控制采集软件及代谢组学软件。

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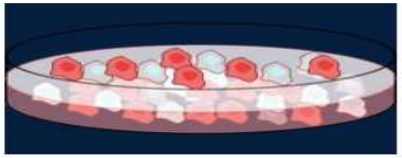
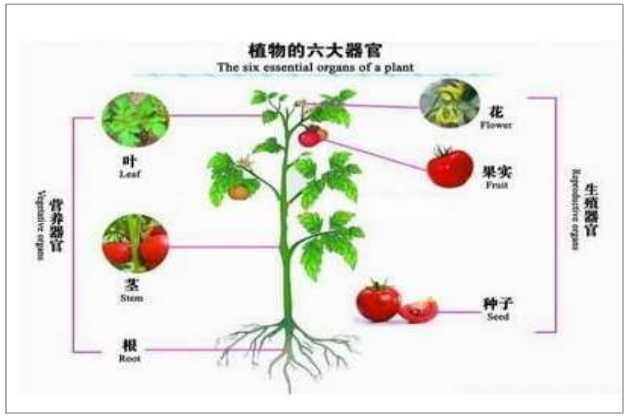
食品安全

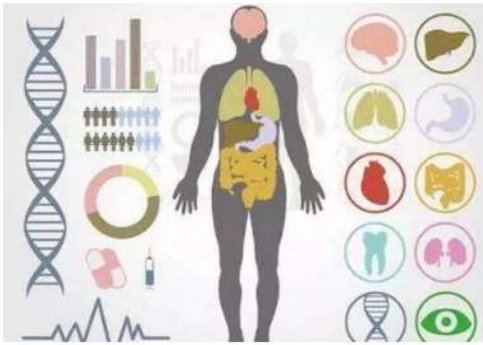
天然产物及功能因子鉴定

未知化合物筛查

代谢组学研究







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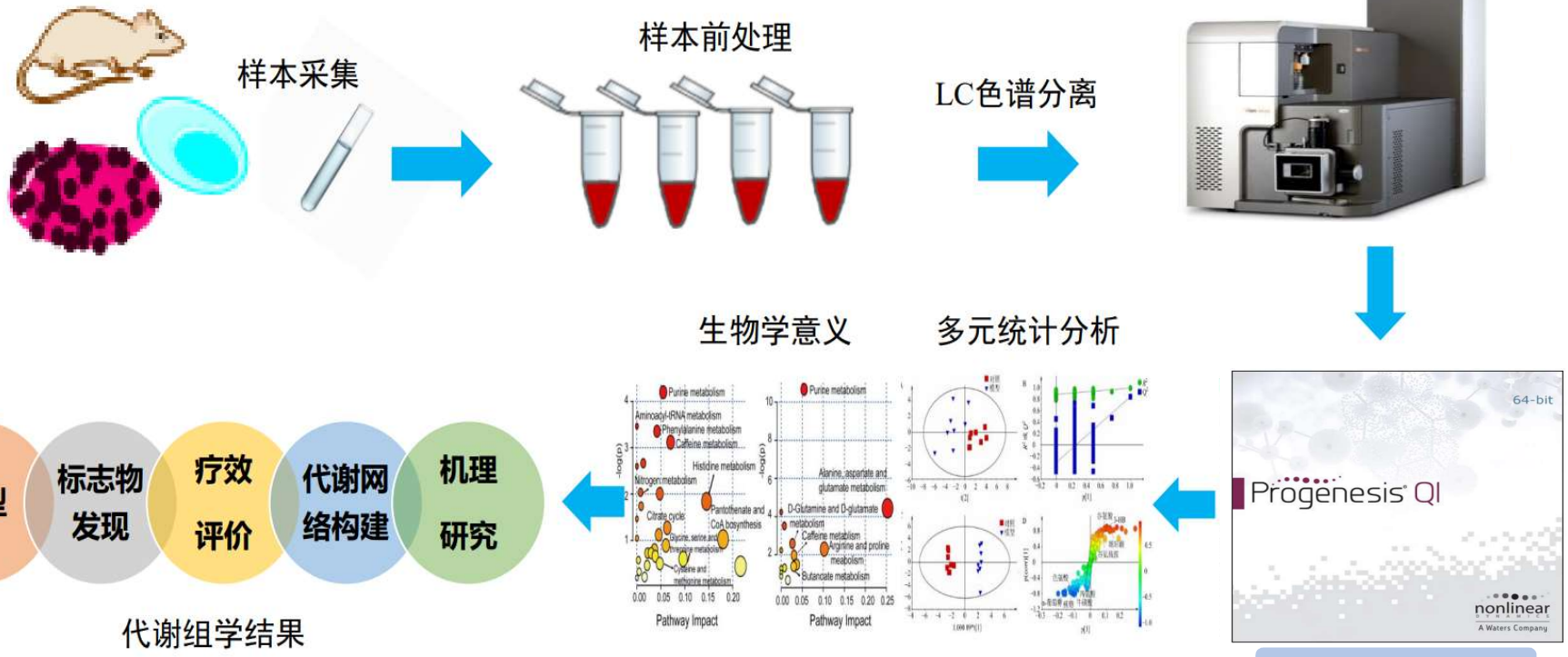
用于代谢组学分析



QI预处理数据

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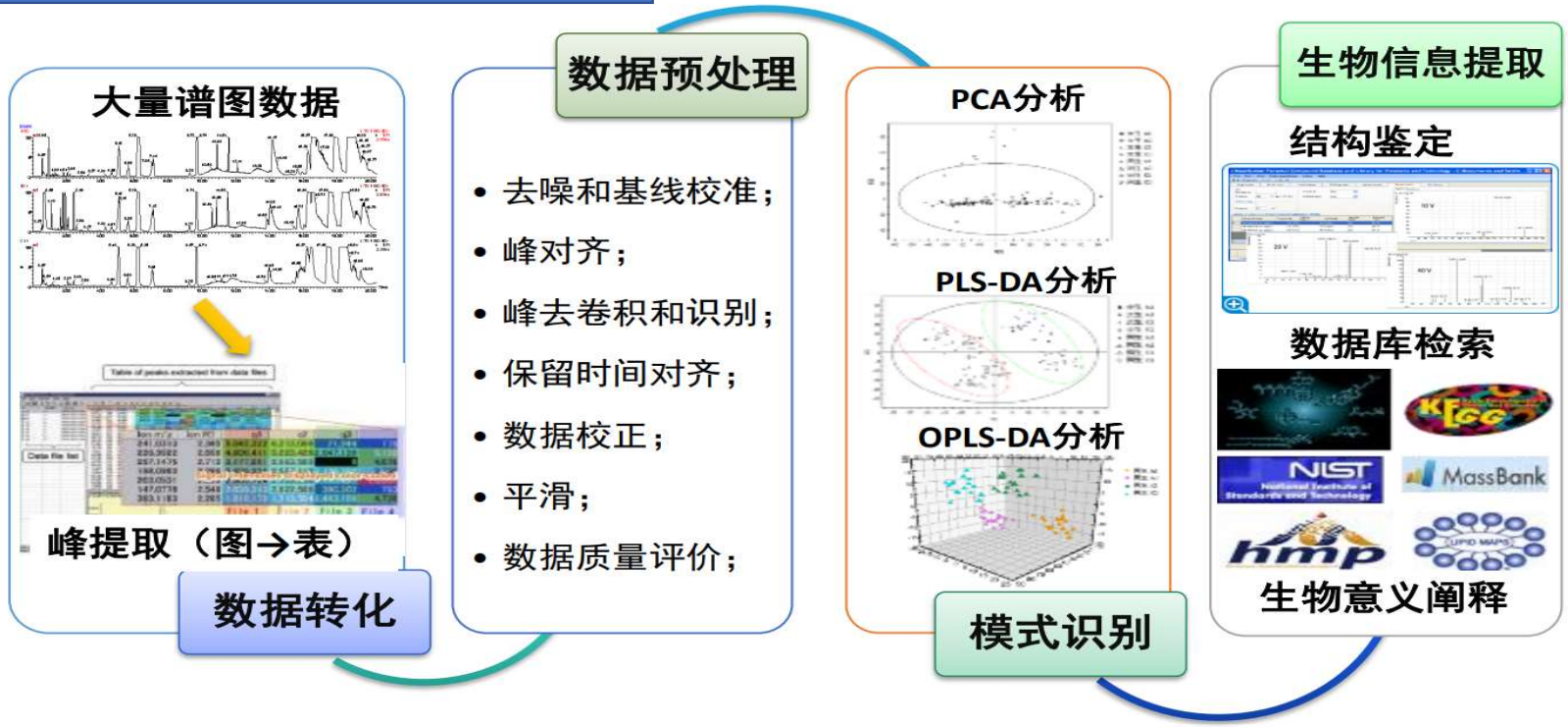
质谱——数据处理全步骤



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QI 处理过程

导入数据
多种格式
1.Waters(.raw)

2.Thermo(.raw)

3.ThermoFT-ICR(.raw)

4.mzXML file

数据对齐
三种模式
1.所有数据源中选择数据对齐参照(**推荐使用**)
2.在指定数据源中选择数据对齐参照
3.在数据源作为对齐参照

试验分组

根据实验分组进行分组即可

峰提取

根据实际情况选择参数

峰去卷积和识别

识别并量化信号，并使之与样品中的代谢物一一对应。

代谢物鉴定

通过数据库鉴定样品中的代谢物。

常用数据库:
HMDB数据库
LIPID MAPS数据库

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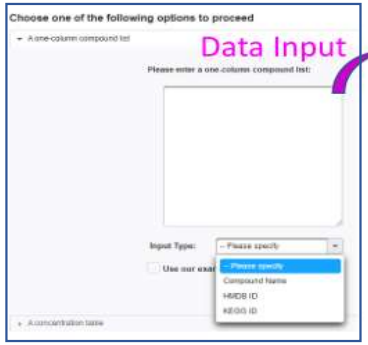
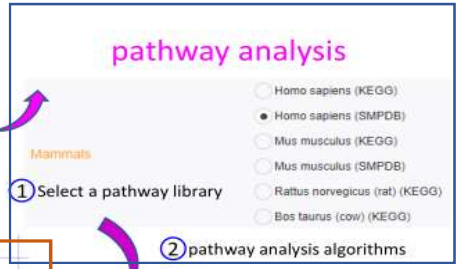
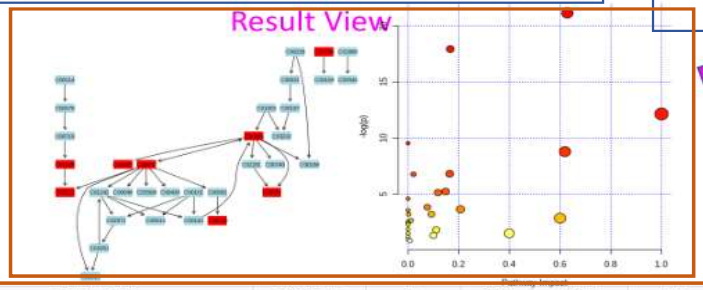
代谢通路分析

QI中鉴定得到得差异代谢物导入KEGG数据库中进行代谢通路分析







Pathway Name	Match Status	p	-log(p)	Holm p	FDR	Impact	Details
Glycine and Serine Metabolism	7/50	1.0079E-5	11.505	9.9786E-4	9.9786E-4	0.11953	KEGG SMP
Methionine Metabolism	6/39	2.9744E-5	10.423	0.0029149	0.0013998	0.11293	KEGG SMP
Phenylalanine and Tyrosine Metabolism	5/25	4.2417E-5	10.068	0.0041145	0.0013998	0.22124	KEGG SMP
Homocysteine Degradation	3/7	1.5995E-4	8.7406	0.015355	0.0039588	0.0	SMP
Ammonia Recycling	3/25	0.0085847	4.7578	0.81554	0.16998	0.0	KEGG SMP
Alanine Metabolism	2/14	0.024105	3.7253	1.0	0.34091	1.0	KEGG SMP
Betaine Metabolism	2/18	0.038852	3.248	1.0	0.42538	0.13201	SMP

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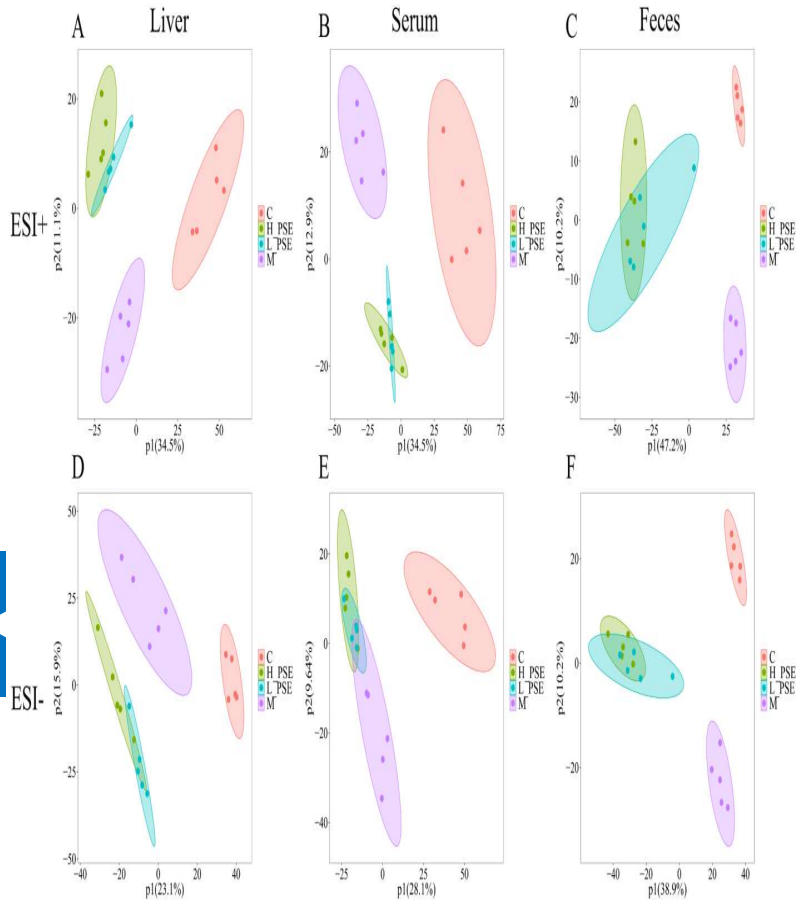
代表性成果1：ApoE$^{-/-}$ 小鼠肝脏、血清和粪便代谢组分析



Title: Peanut skin extract ameliorates high-fat diet-induced atherosclerosis by regulating lipid metabolism, inflammation reaction and gut microbiota in ApoE−/− mice

Journal: Food Research International, If: 7.425

Methods: metabolomics analysis, the raw data obtained from UPLC-Q/TOF-MS were typically pre-processed to provide structured data in an appropriate format for data analysis. First, the raw data were processed by the metabolomics processing software Progenesis **QI software** for baseline filtering, peak identification, integration, retention time correction, peak alignment and normalization.

Result: Different treatment groups could be evidently separated b PLS-DA based on the metabolites in the liver, serum and fecal i both ESI+ and ESI- modes, indicating that there were significar differences in metabolic phenotypes among the experimenta groups.

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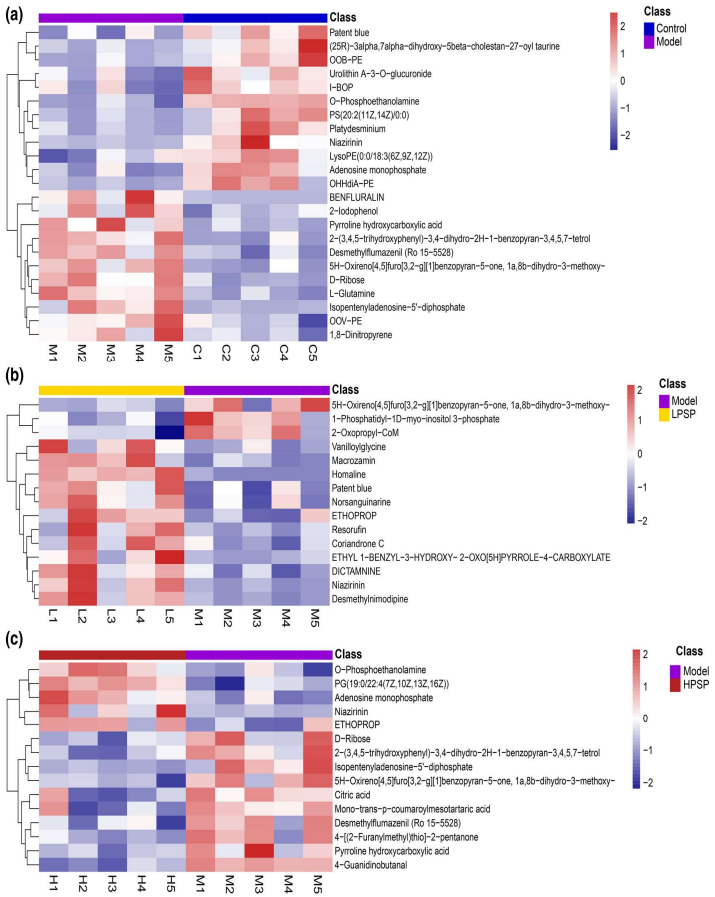
代表性成果II： colitis 小鼠结肠组织代谢组分析

基本信息

主要应用

成果展示



Title: The underlying mechanism of A-type procyanidins from peanut skin on DSS-induced ulcerative colitis mice by regulating gut microbiota and metabolism

Journal: Journal of Food Biochemistry, If: 3.654

Methods: All samples (50 mg) were homogenized together with 20 μL internal standard (2-chloro-l-phenylalanine in methanol, 0.3 mg/mL) and 400μL extraction solvent with methanol /water (4/1, v/v), then vortexed for 1 min. Samples were sonicated for 10 min on ice and then placed at -20 ℃ for 30 min, and then centrifugation at 13,000 rpm for 10 min at 4 ℃. The supernatants were collected for UHPLC-Q-TOF/MS analysis. The metabolome data were processed using Progenesis QI.

Result: A total of 42 different metabolites were identified, and these metabolites indicated that PSP alleviated UC mainly correlated with taste transduction, mTOR signaling pathway, PI3K-Akt signaling pathway, and FoxO signaling pathway

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